Higher order terms in the condensate fraction of a homogeneous and dilute Bose gas

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The condensate fraction of a homogeneous and dilute Bose gas is expanded as a power series of $\sqrt{na^3}$ as $N_0/N = 1 - c_1(na^3)^{1/2} - c_2(na^3) - c_3(na^3)^{3/2}\ldots$. The coefficient c_1 is well-known as $8/3\sqrt{\pi}$, but the others are unknown yet. Considering two-body contact interactions and applying a canonical transformation method twice we developed the method to obtain the higher order coefficients analytically. An iteration method is applied to make up a cutoff in a fluctuation term. The coefficients ares $c_2 = 2(\pi - 8/3)$ and $c_3 = (4/\sqrt{\pi})\,(\pi - 8/3)\,(10/3 - \pi)$.

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I. INTRODUCTION

Homogenous and dilute (HD) Bose gas has been studied for more than a half century since the classical paper by Bogoliubov [1]. Despite its simplicity and significant published research, there still remains some unsolved fundamental problems. The condensate fraction, or the ratio of particles of zero momentum in the perturbed ground state, is a very fundamental concept of a many-body Bose system. At zero temperature, the properties of HD gases are expressed in terms of a single parameter, the s-wave scattering length a, and a quantum loop expansion is expressed by dilute gas parameter $na^3 \ll 1$ where $n = N/V$ is the particle number density.

In a HD system the condensate fraction is expressed as [2, 3]

$$\frac{N_0}{N} = 1 - c_1(na^3)^{1/2} - c_2(na^3) - c_3(na^3)^{3/2} - \ldots. \tag{1}$$

The coefficient c_1 is well-known as $c_1 = 8/3\sqrt{\pi}$, but the others are unknown yet. In this paper, we will calculate the unknown coefficients c_2 and c_3 of the next higher order terms analytically using a double canonical transformation and an iteration method.

II. BOGOLIUBOV HAMILTONIAN

If the interparticle interaction is a contact potential, the effective Hamiltonian for the identical particles of mass m is written as the Bogoliubov form

$$\hat{H} = \sum_k \varepsilon_k a_k^\dagger a_k + \frac{g}{2V} \sum_{\substack{k_1 k_2 \\ k_3 k_4}} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \delta_{k_1+k_2,k_3+k_4}, \tag{2}$$

where $\varepsilon_k = \hbar^2 k^2/2m$ and g is the coupling constant given by $g = 4\pi\hbar^2 a/m$. a_{k_i} and $a_{k_i}^\dagger$ satisfy the bosonic commutator relation: $[a_k, a_{k'}^\dagger] = \delta_{k,k'}$. Note that this Hamiltonian is valid only for the purpose of applying first-order perturbation theory.

Since N_0 is a very large number, the operators a_0 and $a_0^\dagger$ can be regarded as $\sqrt{N_0}$. In a two-body interaction, the interacting part of the Hamiltonian in Eq. (2) is expanded to keep the terms up to the order of N_0^2, N_0, and $\sqrt{N_0}$ as [4, 5, 6]

$$\begin{aligned}
\hat{H}_{int} &= \frac{g}{2V} a_0^\dagger a_0^\dagger a_0 a_0 \\
&+ \frac{g}{2V} \sum_{k\neq 0} \left[2(a_k^\dagger a_0^\dagger a_k a_0 + a_{-k}^\dagger a_0^\dagger a_{-k} a_0) + a_k^\dagger a_{-k}^\dagger a_0 a_0 + a_0^\dagger a_0^\dagger a_k a_{-k} \right] \\
&+ \frac{g}{V} \sum_{k,q\neq 0} \left[a_{k+q}^\dagger a_0^\dagger a_k a_q + a_{k+q}^\dagger a_{-q}^\dagger a_k a_0 \right].
\end{aligned} \tag{3}$$

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The three-body interaction is not considered. The last term, which is generally neglected in textbooks, originates from the interactions of particles out of and into the condensate and the key of the calculation.

Let's introduce a new variable as

$$\gamma_k = \sum_{q\neq 0} a^\dagger_{k+q} a_q. \tag{4}$$

Since the N_0 is expressed by the number relation

$$N_0 = \hat{N} - \frac{1}{2}\sum_{k\neq 0}(a^\dagger_k a_k + a^\dagger_{-k} a_{-k}), \tag{5}$$

we can rewrite the model Hamiltonian as a function of the density n as

$$\begin{aligned} \hat{H} &= \frac{1}{2}n^2 V g \\ &+ \frac{1}{2}\sum_{k\neq 0}\Big[(\varepsilon_k + ng)(a^\dagger_k a_k + a^\dagger_{-k}a_{-k}) + ng(a^\dagger_k a^\dagger_{-k} + a_k a_{-k})\Big] \\ &+ \frac{ng}{\sqrt{N}}\sum_{k\neq 0}\gamma_k (a_k + a^\dagger_{-k}). \end{aligned} \tag{6}$$

III. DOUBLE CANONICAL TRANSFORMATION

Next, we apply the conventional Bogoliubov transformation of the new the operators a_k and $a^\dagger_k$ to diagonalize the Hamiltonian [1].

$$\begin{aligned} a_k &= \frac{1}{\sqrt{1-A_k^2}}(b_k + A_k b^\dagger_{-k}), \\ a^\dagger_k &= \frac{1}{\sqrt{1-A_k^2}}(b^\dagger_k + A_k b_{-k}). \end{aligned} \tag{7}$$

It is clear that b_k and $b^\dagger_k$ satisfy the same commutator relations as a_k and $a^\dagger_k$. Then, the Hamiltonian in Eq. (6) becomes

$$\begin{aligned} \hat{H} &= \frac{1}{2}n^2 V g + \sum_{k\neq 0}\frac{1}{1-A_k^2}\left[(\varepsilon_k + ng)A_k^2 + ngA_k\right] \\ &+ \frac{1}{2}\sum_{k\neq 0}\frac{1}{1-A_k^2}\left[(\varepsilon_k+ng)(1+A_k^2) + 2ngA_k\right](b^\dagger_k b_k + b^\dagger_{-k}b_{-k}) \\ &+ \frac{1}{2}\sum_{k\neq 0}\frac{1}{1-A_k^2}\left[2(\varepsilon_k+ng)A_k + ng(1+A_k^2)\right](b^\dagger_k b^\dagger_{-k} + b_k b_{-k}) \\ &+ \frac{ng}{\sqrt{N}}\sum_{k\neq 0}\frac{(1+A_k)}{\sqrt{1-A_k^2}}(b_k + b^\dagger_{-k})\gamma_k. \end{aligned} \tag{8}$$

A_k is chosen to make the off-diagonal term vanish.

$$2(\varepsilon_k + ng)A_k + ng(1+A_k^2) = 0, \tag{9}$$

and we obtain $A_k (= A_{-k})$ as

$$A_k = \frac{E_k - (\varepsilon_k + ng)}{ng}, \tag{10}$$

where

$$E_k = \sqrt{(\varepsilon_k + ng)^2 - (ng)^2}. \tag{11}$$

The E_k is the Bogoliubov form of the dispersion relation.

Substituting A_k into the Hamiltonian in Eq. (8), we obtain the following compact form of the Hamiltonian

$$\begin{aligned}\hat{H} &= \frac{1}{2}n^2Vg + \sum_{k\neq 0}\frac{1}{1-A_k^2}\left[(\varepsilon_k+ng)A_k^2+ngA_k\right] \\ &+ \sum_{k\neq 0}E_k b_k^\dagger b_k + \sum_{k\neq 0}G_k(b_k+b_{-k}^\dagger),\end{aligned} \tag{12}$$

where

$$G_k = \frac{ng}{\sqrt{N}}\frac{(1+A_k)\gamma_k}{\sqrt{1-A_k^2}}. \tag{13}$$

The first three terms in the right hand side of Eq. (12) are already known and the last one is the new contribution beyond the textbook results [2, 3, 4]. We can regard the system as a collection of quantum mechanical harmonic oscillators exposed to additional forces given by linear terms. The linear terms b_k and $b_k^\dagger$ can be made to eliminate by another linear transformation of the form

$$\begin{aligned} b_k &= c_k + \alpha_k, \\ b_k^\dagger &= c_k^\dagger + \alpha_{-k},\end{aligned} \tag{14}$$

where the new operators c_k and $c_k^\dagger$ satisfy the bosonic commutator relations. Note that α_k commutes with c_k and $\alpha_k^\dagger = \alpha_{-k}$ since b_k and $b_k^\dagger$ are bosonic operators.

Substituting the new operators in Eq. (14) into Eq. (12), we can rewrite the Hamiltonian in Eq. (12) as

$$\begin{aligned}\hat{H} &= \frac{1}{2}n^2Vg + \sum_{k\neq 0}\frac{1}{1-A_k^2}\left[(\varepsilon_k+ng)A_k^2+ngA_k\right] \\ &+ \sum_{k\neq 0}\left(E_k c_k^\dagger c_k + E_k\alpha_{-k}\alpha_k + 2G_k\alpha_k\right) \\ &+ \sum_{k\neq 0}\left[(E_k\alpha_{-k}+G_k)c_k + (E_k\alpha_k + G_{-k})c_k^\dagger\right].\end{aligned} \tag{15}$$

We choose α_k to make the linear terms vanish as

$$\alpha_k = -\frac{G_{-k}}{E_k}. \tag{16}$$

Then, the Hamiltonian in Eq. (15) is now diagonalized in terms of the new operators as follows

$$\begin{aligned}\hat{H} &= \frac{1}{2}n^2Vg + \sum_{k\neq 0}\frac{1}{1-A_k^2}\left[(\varepsilon_k+ng)A_k^2+ngA_k\right] - \sum_{k\neq 0}\frac{G_kG_{-k}}{E_k} + \sum_{k\neq 0}E_k c_k^\dagger c_k \\ &= \hat{H}_g + \sum_{k\neq 0}E_k n_k.\end{aligned} \tag{17}$$

$\hat{H}_g$ creates the well-known ground state energy density [2, 3, 4] but we will not discuss it here.

$$\frac{E_g}{V} = \frac{2\pi\hbar^2 an^2}{m}\left[1 + \frac{128}{15}\left(\frac{na^3}{\pi}\right)^{1/2} + \dots\right]. \tag{18}$$

IV. CONDENSATE TRACTION

The condensate fraction is defined as $(N - \sum_{k\neq 0} n_k)/N$. We obtain the particle distribution n_k of the dilute system from Eqs. (7) and (14) as

$$\begin{aligned} n_k &= \langle 0|a_k^\dagger a_k|0\rangle \\ &= \frac{A_k^2}{1-A_k^2} + \frac{(1+A_k)^2}{1-A_k^2}\langle 0|\alpha_{-k}\alpha_k|0\rangle \\ &= \frac{1}{2}\left(\frac{\varepsilon_k+ng}{E_k} - 1\right) + \frac{1}{N}\frac{n^2g^2\varepsilon_k^2}{E_k^4}\langle 0|\gamma_k\gamma_{-k}|0\rangle.\end{aligned} \tag{19}$$

Note that $(1+A_k)/(1-A_k) = \varepsilon_k/E_k$. The magnitude of $ng\varepsilon_k/E_k^2$ is order of 1. The first term is shown in the textbooks and produces the well-known c_1 in Eq. (1). On the other hand, the relation between the second term and n_k will create c_2.

The dominant part of the unknown quantity $\langle 0|\gamma_k\gamma_{-k}|0\rangle$ is obtained in the following way. Applying the definition of γ_k in Eq. (4), the ground state average is written as

$$\langle 0|\gamma_k\gamma_{-k}|0\rangle = \langle 0|\sum_{q,q'\neq 0} a^\dagger_{k+q}a_q a^\dagger_{-k+q'}a_{q'}|0\rangle. \tag{20}$$

The summation is composed of the two terms as $\sum_{q,q'\neq 0} = \sum_{q'=k+q} + \sum_{q'\neq k+q}$. It is known that the dominant contribution arises when a particle interacts with itself and it belongs to the term $\mathbf{q}' = \mathbf{k}+\mathbf{q}$. Then, we can separate the dominant contribution into two parts $\mathbf{q} = \mathbf{q}'$ and $\mathbf{q} \neq \mathbf{q}'$ again, but the term for $\mathbf{q} \neq \mathbf{q}'$ vanishes using the argument of random phase approximation. Therefore, we have

$$\begin{aligned}\langle 0|\gamma_k\gamma_{-k}|0\rangle &\simeq \langle 0|\sum_{q'=k+q} a^\dagger_{k+q}a_q a^\dagger_{-k+q'}a_{q'}|0\rangle \\ &= \langle 0|\sum_{q=q'\neq 0} a^\dagger_{q'}a_q a^\dagger_{q}a_{q'}|0\rangle + (k\text{−dependent minor terms}).\end{aligned} \tag{21}$$

Within this approximation, using the n_k in Eq. (19), we can write Eq. (21) as

$$\begin{aligned}\langle 0|\gamma_k\gamma_{-k}|0\rangle &\simeq \sum_{q\neq 0} n_q^2 \\ &= \sum_{q\neq 0}\left[\frac{1}{2}\left(\frac{\varepsilon_q+ng}{E_q}-1\right)\right]^2 + (k\text{−dependent minor terms}) \\ &= N\left[\left(\pi-\frac{8}{3}\right)\eta + \mathcal{O}(\eta^2)\right],\end{aligned} \tag{22}$$

where $\eta = \sqrt{na^3/\pi} \ll 1$. We put $\hbar = m = 1$, and $\sum_q = (N/2\pi^2 n)\int q^2 dq$ for convenience. The cutoff of the k-dependent minor terms is at most order of η^2 or smaller. The effective range of the cutoff is judged the by an iteration method self-consistently.

Substituting $\langle 0|\gamma_k\gamma_{-k}|0\rangle$ in Eq. (22) into Eq. (19), we obtain a new higher order n_k as

$$n_k = \frac{1}{2}\left(\frac{\varepsilon_k+ng}{E_k}-1\right) + \left(\pi-\frac{8}{3}\right)\frac{n^2g^2{\varepsilon_k}^2}{E_k^4}\eta + \mathcal{O}(\eta^2). \tag{23}$$

Now, let us back the new n_k into Eq. (22) to obtain a new higher order $\langle 0|\gamma_k\gamma_{-k}|0\rangle$, too.

$$\begin{aligned}\langle 0|\gamma_k\gamma_{-k}|0\rangle &= \sum_{q\neq 0}\left[\frac{1}{2}\left(\frac{\varepsilon_q+ng}{E_q}-1\right) + \left(\pi-\frac{8}{3}\right)\frac{n^2g^2{\varepsilon_q}^2}{E_q^4}\eta + \mathcal{O}(\eta^2)\right]^2 \\ &= N\left[\left(\pi-\frac{8}{3}\right)\eta + 2\left(\pi-\frac{8}{3}\right)\left(\frac{10}{3}-\pi\right)\eta^2 + \frac{\pi}{16}\left(\pi-\frac{8}{3}\right)^2\eta^3 + \mathcal{O}(\eta^3)\right].\end{aligned} \tag{24}$$

Therefore, we can trust up to η^2 term in $\langle 0|\gamma_k\gamma_{-k}|0\rangle$ with the cutoff.

Finally, substituting Eq. (24) into Eq. (19), we obtain the next higher order two coefficients c_2 and c_3. The particle depletion from the zero momentum condensate, $(N-N_0)/N$, is

$$\begin{aligned}\frac{1}{N}\sum_{k\neq 0} n_k &= \frac{1}{2N}\sum_{k\neq 0}\left(\frac{\varepsilon_k+ng}{E_k}-1\right) + \frac{1}{N}\sum_{k\neq 0}\frac{n^2g^2{\varepsilon_k}^2}{E_k^4}\left[\left(\pi-\frac{8}{3}\right)\eta + 2\left(\pi-\frac{8}{3}\right)\left(\frac{10}{3}-\pi\right)\eta^2 + \mathcal{O}(\eta^3)\right] \\ &= \frac{8}{3}\eta + 2\pi\left(\pi-\frac{8}{3}\right)\eta^2 + 4\pi\left(\pi-\frac{8}{3}\right)\left(\frac{10}{3}-\pi\right)\eta^3 + \mathcal{O}(\eta^4) \\ &= \frac{8}{3\sqrt{\pi}}(na^3)^{1/2} + 2\left(\pi-\frac{8}{3}\right)na^3 + \frac{4}{\sqrt{\pi}}\left(\pi-\frac{8}{3}\right)\left(\frac{10}{3}-\pi\right)(na^3)^{3/2} + \mathcal{O}((na^3)^2).\end{aligned} \tag{25}$$

Therefore, finally, we obtain $c_2 = 2(\pi - 8/3)$ and $c_3 = (4/\sqrt{\pi})\,(\pi - 8/3)\,(10/3 - \pi)$.

V. SUMMARY

We expanded the Hamiltonian of a homogeneous and interacting Bose system up to the $\sqrt{N_0}$ terms, and applied the canonical transformation twice to find the average value of the higher order terms. An iteration method was applied to make up the cutoff. Two higher order coefficients c_2 and c_3 were obtained analytically.

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